WP PWIE meeting, 24-27. March 2025



Influence of the kinetic energy of the exposing species on deuterium uptake in tungsten

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This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

Basic idea of the experiment





- Study permeation in W foil with D species having different kinetic energy at different temperatures
- Surface processes vs.
 direct implantation

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- Study permeation in W foil with D species having different kinetic energy at different temperatures
- Surface processes vs. direct implantation

- Measurement of D uptake in 2 μm self-damaged W layer of the permeating D as function of D atom/ion fluence [B. Tyburska et al. JNM 415 (2011) S680–S683]
- To prevent D atom or molecule on the downstream side an additional protective Al₂O₃ layer with an Ag spacer was deposited on the damaged side.

Experimental set up



- ✓ Sample preparation procedure = 50 µm W foil (Goodfellow)
 ✓ Recrystalized
- ✓ 20 MeV W irradiation at 290 K to a fluence of 7.8e17 W/m2 –
 0.23 dpa in peak maximum
- ✓ Protective Al₂O₃ (85 nm) layer with Ag (1 µm) spacer (deposited by A. Manhard/MPG by magnetron sputtering following the procedure by [Kapser et al. NME 12 (2017) 703– 708.)
- ✓ Sample mounted on a home-made heater (copper plate with embedded two filament heater) with a central hole for ion beam analysis.





Experimental set up



Upstream side: <u>Exposure</u> to D atoms of 0.3 eV energy or D ions with 300 eV energy at 600 K and 700 K foil temperature.

Downstream side: <u>In situ analysis by Nuclear</u> <u>Reaction analysis (NRA)</u> using ³He beam from 2 MV Tandem accelerator on the side where displacement damage layer by 20 MeV W ions was created with protective layer on top



 ✓ Good separation of D in Al₂O₃ and in W damaged layer





Results: D permeation through W with 300 eV/D ions

D ion exposure

- Experiment
- ✓ Exposure to **D** ions (flux 8e18 D/m²) for ~ 600/700 K for ~ 75 h/ 96h

- \checkmark Measured D depth profiles on the downstream side
- <u>Ions</u> Surprise: No diffusion front visible but raising D concentration within damaged layer



Results: D permeation through W with 0.3 eV D atoms

D atom exposure

- Section 2 Constrained Section 2 Constrain
- Exposure to D atoms (flux 5e18 D/m²) at 600/700 K for ~ 160 h/ 250 h

- ✓ Measured D depth profiles on the downstream side
- <u>Atoms</u>: Very low concentration and also 'constant' D concentration through the damaged layer different compared to the depth profile measured at direct uptake of self-damaged W





For comparison direct D uptake in self-damaged layer

Results: Comparison of D permeation through W with D atoms and 300 eV/D ions



Section 2 Sec

Éxposure to
 D atoms at 600/700 K for ~ 160 h/ 250 h
 D ions for ~ 600/700 K for ~ 75 h/ 96h

- Very short "lag time" in all cases
- Ions: slower increase at 700 K
- Atoms: very slow faster at 700 K
- Reverse behavior ions versus atoms thermal detrapping – surface barrier
- For interpretation we need macroscopic rate equation (MRE) modelling





Modelling: D permeation through W foil

Self-damaged layers

3 traps [M. Pečovnik *et al*, Nucl. Fusion 60 (2020)]: **Trap 1:** $E_{dt} = 1.46 - 1.08 \text{ eV}$ (5 levels), lons or $n_{\rm t} = 0.140 \ (600 \ {\rm K}) - 0.105 \ (700 \ {\rm K}) \ {\rm at.\%}$ atoms **Trap 2:** $E_{dt} = 1.86 - 1.68 \text{ eV}$ (2 levels), $n_{\rm t} = 0.140 \ (600 \ {\rm K}) - 0.125 \ (700 \ {\rm K}) \ {\rm at.\%}$ **Trap 3:** $E_{dt} = 2.05 \text{ eV}, n_t = 0.050 \text{ at.}\%$ Defect annealing – D concentration decrease at Using $D_{\rm H}(T) = 1.9 \times 10^{-7} \exp\left(-\frac{0.2 \text{ eV}}{k_{\rm P}T}\right) \text{m}^2\text{s}^{-1}$ (DFT calculations from [Fernandez et al, Acta Mater. 94 (2015)]

Boundary conditions on the exposed surface:

Surface model parameters for atoms and also for ions [Hodille et al, Nucl. Fusion 60 (2020)] Including sputtering of adsorbed D by high energy ions [Hodille et al, Nucl. Fusion 64 (2024) 046022] with $Y_{\rm sput} = 3$

No Desorption at the back surface (to simulate the alumina layer)







Modelling: Boundary conditions

lons or





Hodille et al, Nucl Fusion 60 (2020) 106011

Kinetic surface model: $dc_{\rm surf}$

$$\frac{dt}{dt} = F_{\text{in}} - F_{\text{out}} + F_{\text{surf}\leftrightarrow\text{bulk}}$$
$$\lambda \frac{dc_{\text{m}}}{dt} = -F_{\text{surf}\leftrightarrow\text{bulk}} - F_{\text{diff}}$$

W

Abstraction by atoms: $\sigma_{\rm abs} = 1.7 \times 10^{-21} \, {\rm m}^2$

Hodille et al, Nucl Fusion 60 (2020) 106011

Abstraction (sputtering) by ions: $Y_{\rm sput} = 3.0 \text{ or } \sigma_{\rm sput} = 2.7 \times 10^{-20} \text{ m}^2$

Hodille et al, Nucl Fusion 64 (2024) 046022

damaged No flux conditions: $\frac{\partial c_m}{\partial x} = 0$

 AI_20_3



Modelling: D permeation through W foil



W-irradiated area



- Using $D_{\rm H}(T) = 1.9 \times$ • $10^{-7} \exp\left(-\frac{0.2 \text{ eV}}{k_{\text{B}}T}\right) \text{m}^2\text{s}^{-1}$ (DFT calculations from [Fernandez et al, Acta Mater. 94 (2015)]
- ✤ 600 K: wrong D depth profile behaviour ⇒ two diffusion channels ? (Grain Boundaries)



0.00

46.0

46.5

47.0

47.5

48.0

Depth (µm)

48.5

49.0

49.5

50.0







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Modelling: D permeation through W foil

In both simulation and experiment the same temperature behaviour: lons: Ret(600 K)>Ret(700K) Atoms: Ret(600K)<Ret(700K)

- It is temperature (T) dependent:
 - because of solute concentration changes with T Increases with T for atoms, decreases for ions
 - damage concentration decreases due to annealing (700 K), higher detrapping







- Higher diffusion coefficient than from DFT [Fernandez *et al*, Acta Mater. 94 (2015)] Ediff=0.2 eV or recent measurements [Holzner, G., Phys. Scr. T171, 014034 (2020).] Ediff=0.28 eV
- Obtained effective diffusion values





H-prefiling - basic idea of the experiment with





Study D uptake but with Hprefiling

- H-prefilling to decorate the deep traps in the foil
- Faster transport for subsequent D

Uptake in H pre-filled W foil at 600 K



Idea: filling the deep traps by H atoms, is then diffusion faster?

H pre-filled W foil: First H ion exposure and second D ion exposure

Experiment

Exposure scenario:

- 1. H ions 24 h (flux 5e18 D/m²) at 600 K for
- 2. D ions (flux 6e18 D/m²) at 600 K for ~ 50 h
- Exposure of recrystallized foil and stress relieved foil (heating to 1200 K)

Observations

 Difference in D retention between recrystallized foil and stress relieved foil?

D depth profiles – lons at 600 K; Comparison prefilled with H ions and no H-prefill



Idea: filling the deep traps by H atoms, is then diffusion faster?

H pre-filled W foil: First H ion exposure and second D ion exposure

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- 2. D ions (flux 6e18 D/m²) at 600 K for ~ 50 h
- Exposure of recrystallized foil and stress relieved foil (heating to 1200 K)

Observations

- Difference in D retention between recrystallized foil and stress relieved foil?
- After 24 of exposure the D retention is more than
 4 times higher compared to no pre-filling with H

D uptake – H pre-filled W foil (with H ions)



Uptake in H pre-filled W foil at 400 K



Study of D permeation in H-prefilled W foil at low temperatures through W foil with 300 eV/D ions

<u>400 K case</u>

Experiment

- Exposure of stress-relieved 50 μ m W foils with protective layer Al₂O₃
- 1. Exposure to H ions (flux $3x10^{18}$ H/m²s) at 600 K for 24h
- 2. Exposure to D ions at 400 K; flux 2.7x10¹⁸ D/m2s

- ✓ After 96 h the NRA signal the same as after 4 h
- No observable D uptake at 400 K even after H prefilling at 600 K to saturate the deep traps
- Graph shows comparison to previous exposures at 600 K and 700 K



Uptake in H pre-filled W foil at 500 K

- Study of D permeation in H-prefilled W foil at low temperatures through W foil with 300 eV/D ions

500 K case

Experiment

- Exposure of <u>stress-relieved 50 µm</u> W foils with protective layer Al₂O₃
- Exposure to H ions (flux 3x10¹⁸ H/m²s) at 600 K for 24h
- 2. Exposure to D ions at 500 K; flux 2.7x10¹⁸ D/m2s

- ✓ After 46 h the NRA signal started to increase different position on the foil (factor of 6 in D signal change from one position to another)
- Comparison to previous exposures at 600 K and 400 K without and with H-prefilling



Permeation at 400 K and 500 K

Study of D permeation in H-prefilled W foil at low temperatures through W foil with 300 eV/D ions

0.4

D concentration [at. %]

Experiment

- Exposure of stress-relieved 50 μ m W foils with protective layer Al₂O₃
- Exposure to H ions (flux 3x10¹⁸ H/m²s) at 600 K for 24h
- 2. Exposure to D ions at 500 K; flux 2.7x10¹⁸ D/m2s

- D depth profile shows filling of the W foil from the backside
- Very variable D signal over the W foil Last depth profile measured at maximum D signal (grain boundaries?)









Influence of surface kinetics on D uptake

- Assuming similar fluences ion permeation faster
- Temperature effect faster at 700 K for atoms influence of surface barrier
 - slower at 700 K for ions thermal detrapping / damage annealing
- H-prefiling does promote faster uptake

Future

- Macroscopic rate equation modeling Suggestion of new model including 2 diffusions path (grain boundaries ?) - the implementation of such model started
- Permeation in stress relieved foil versus recrystallized grains micrometer size for D atoms at 600 K – influence of grain boundary diffusion



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